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Swiss Federal Institute of Technology Zurich

VisTrails Introduction

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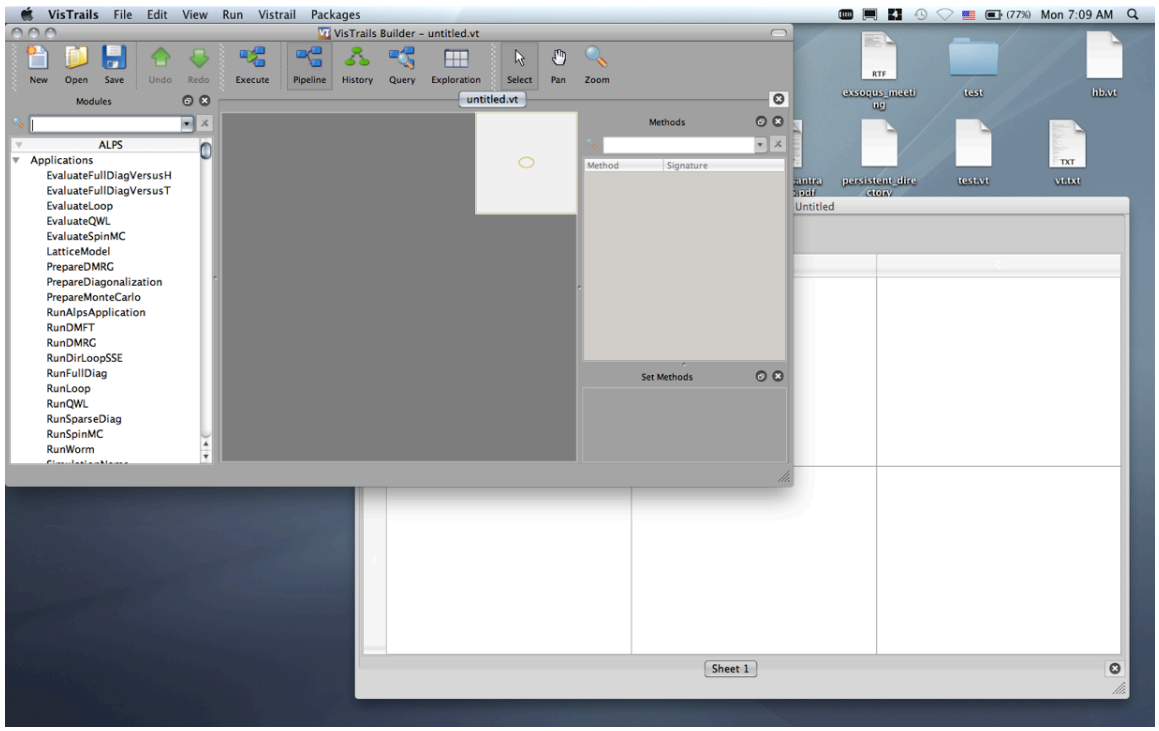
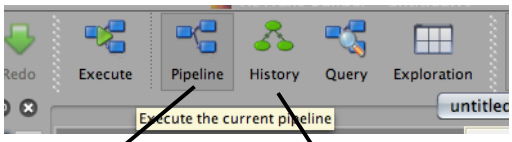
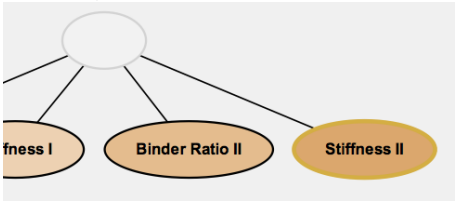
Vistrails windows



Views



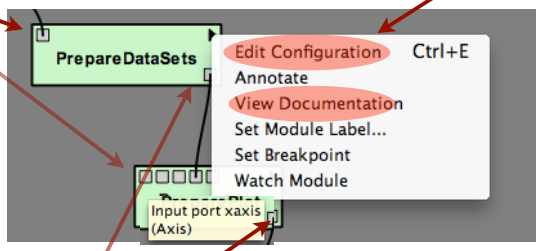


Modules

Important for source modules!

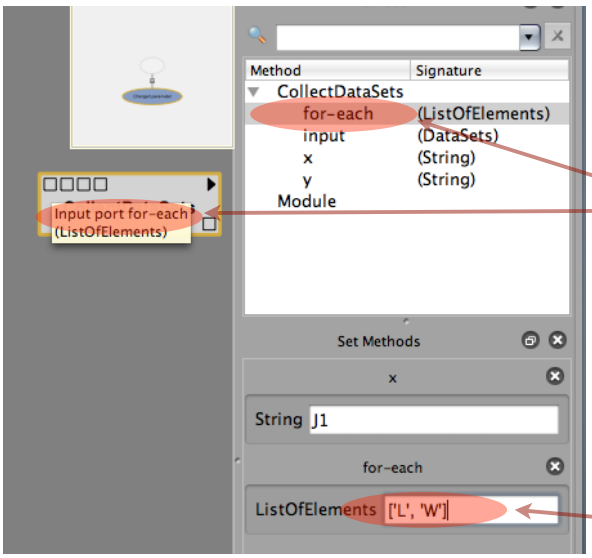
Input ports

Ports:
- Input/Output
- Name
- Type:
  - VT module class
  - Connects only matching types
  - Weak typing



Output ports

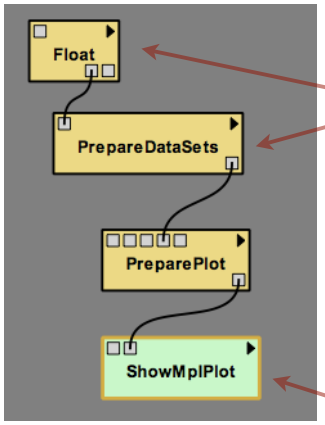
More on modules



Input ports can often be set from other modules or directly

Most types are entered in the syntax of the Python interpreter!

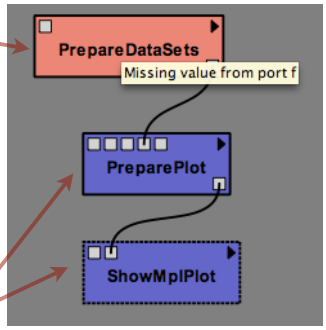
Pipeline execution



Cached

Executed

Error

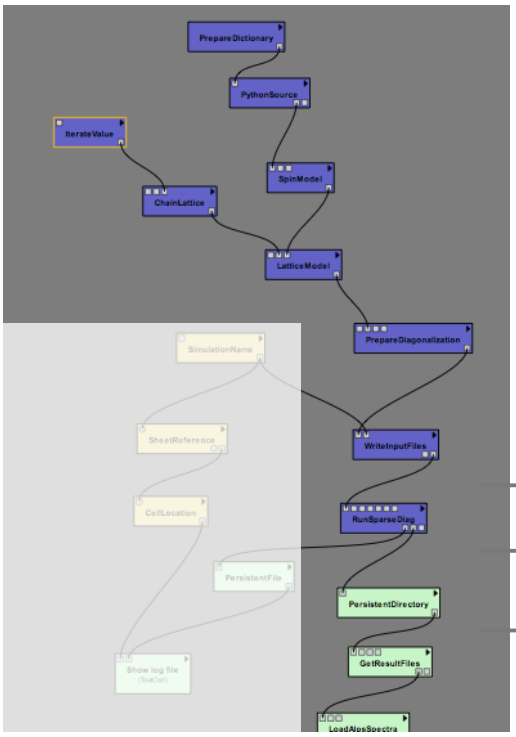


Not executed

Caching

- Memory caching
  - Fully automatic
  - Lost after restarting VisTrails
- Disk caching (*persistent cache*)
  - Needs to be enabled by user
  - Remains "forever"
  - `PersistentFile`/`PersistentDirectory` modules

Persistence



Input preparation

Running the simulation

Storing to persistence

Data analysis

More persistence

- Where does it go?
  - ~/.vistrails/persistent_files
- Other locations can be set in Preferences

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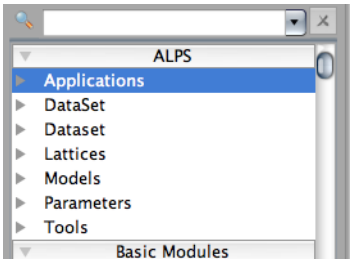
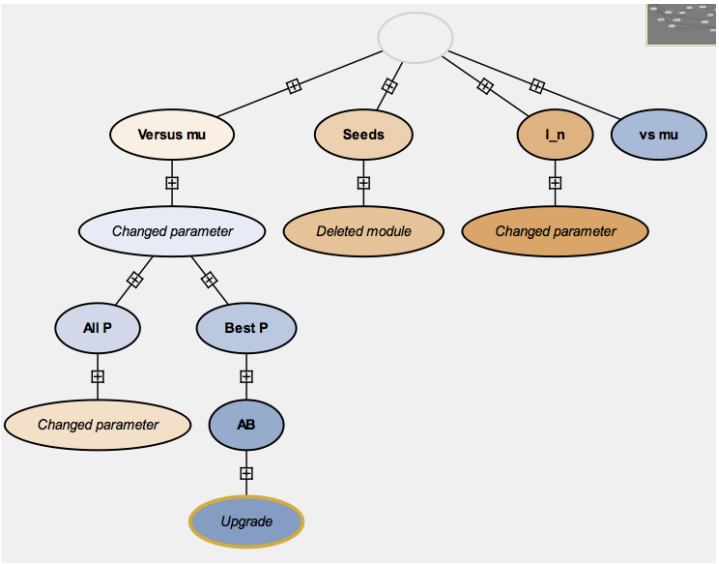
ALPS modules

- Library/applications-related modules
  - Gives access to ALPS applications with preparation of models, lattices, etc.
  - Closely related: Parameters modules



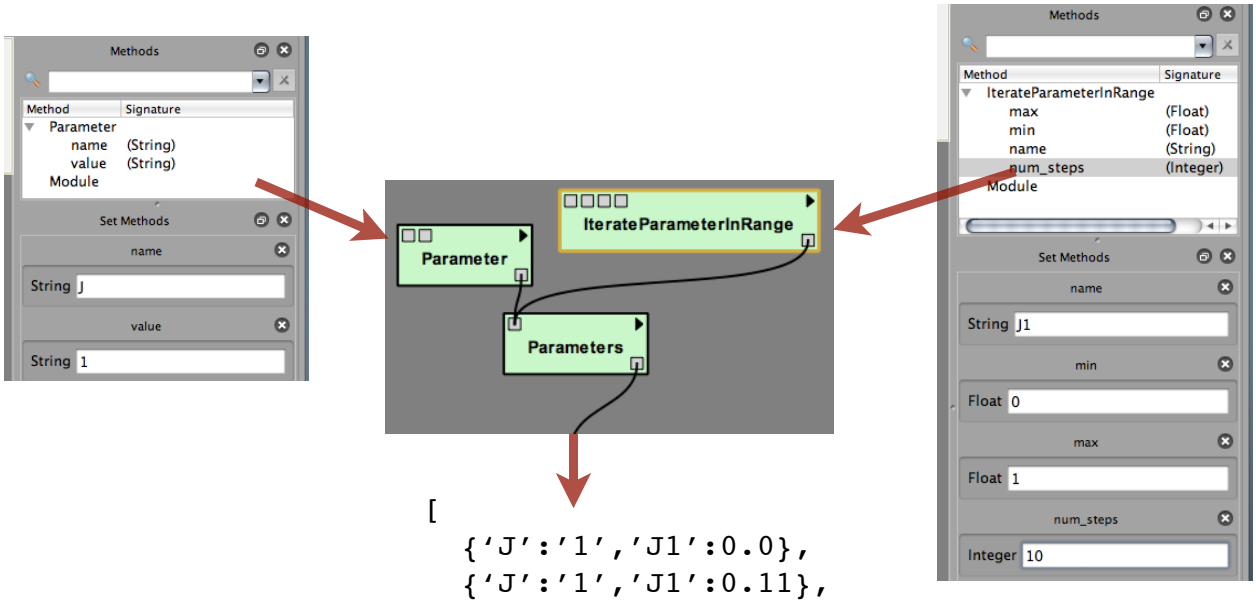
- DataSet modules
  - Independent of ALPS library and applications
  - 'Scriptable plotting and data analysis tool'

History



- Instead of separate files, you can maintain branches in the history
- Undo in the Pipeline means going up in History
- No Undo in History: once you delete a branch, it's gone for good!

Setting up parameters




```
[
  {'J':'1','J1':0.0},
  {'J':'1','J1':0.11},
  ...
]
```

DataSet modules

- DataSet synopsis:

```
class DataSet:
    def __init__(self):
        self.x = np.array([])
        self.y = np.array([])
        self.props = {}
```

- `x/y` should contain data, `props` should be a dictionary containing all information about the data
- DataSet modules exchange lists of DataSets
- Most modules will imply loop over all entries in the list

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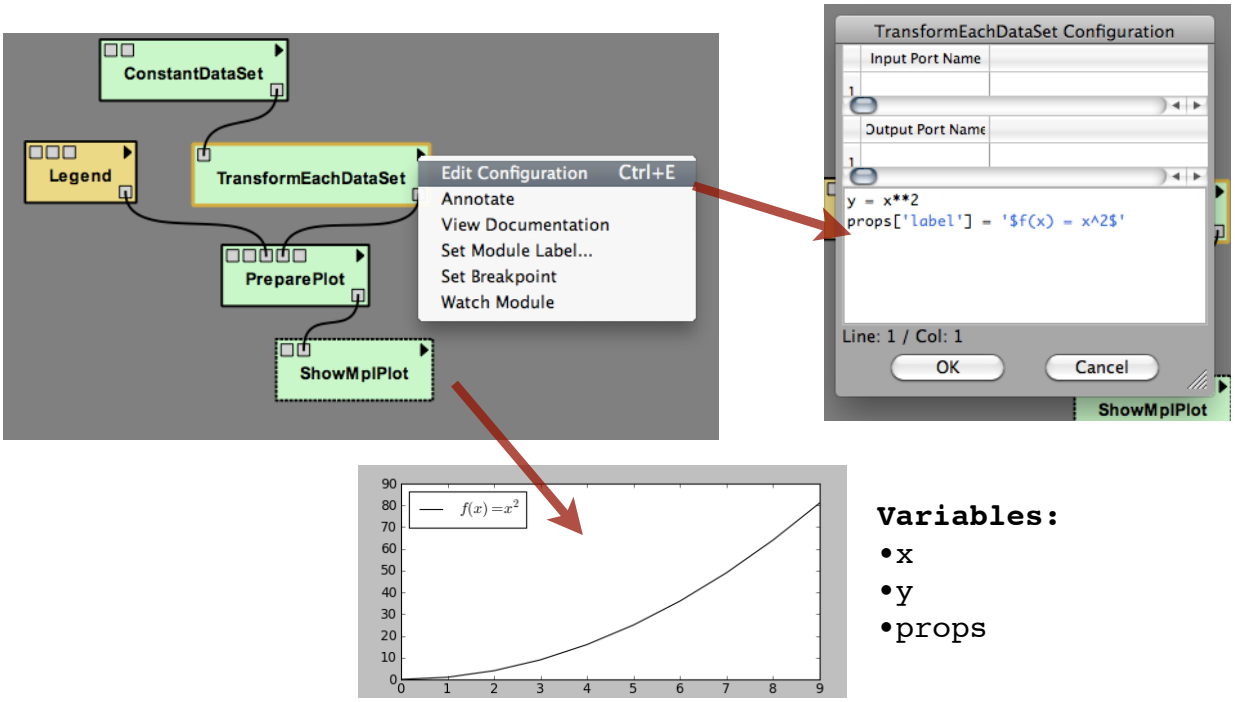
More on DataSets

- Transform modules allow arbitrary operations
- Plotting tools will read information (labels, line colors/type, ...) from props, including
  - `'label'`, `'line'`, `'linewidth'`, `'xlabel'`/`'ylabel'`, `'marker'`, `'markersize'`
- Error bars will be shown if data type has mean/error members
  - Such data types that support error propagation in calculations are part of `pyalps.pyalea`

A simple workflow



Variables:

- x
- y
- props

Hierarchical datasets

- Problem: find minimal energy for each `t` in the list

```
[(x=[],y=[],props={t:1,V:1}),
 (x=[],y=[],props={t:1,V:2}),
 (x=[],y=[],props={t:2,v:1}),
 (x=[],y=[],props={t:2,V:2})]
```

- In a flat list: cumbersome

```
mins = {}
for ds in data:
    if ds.props[t] in mins:
        mins[ds.props[t]] = min(min(ds.y), mins[ds.props[t]])
    else:
        mins[ds.props[t]] = min(ds.y)
```

Hierarchical datasets

- Consider hierarchical list

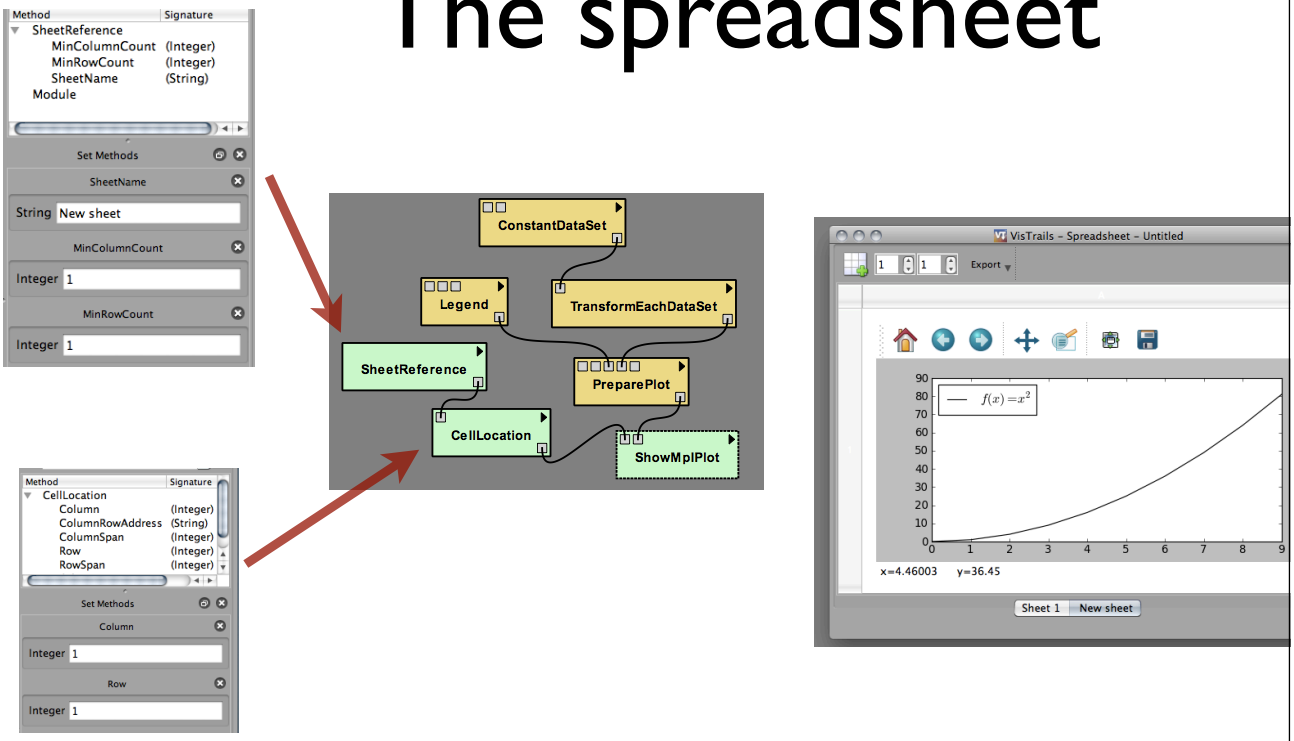
```
[[(x=[],y=[],props={t:1,V:1}),
  (x=[],y=[],props={t:1,V:2})],
 [(x=[],y=[],props={t:2,v:1}),
  (x=[],y=[],props={t:2,V:2})]]
```

- Much easier now:

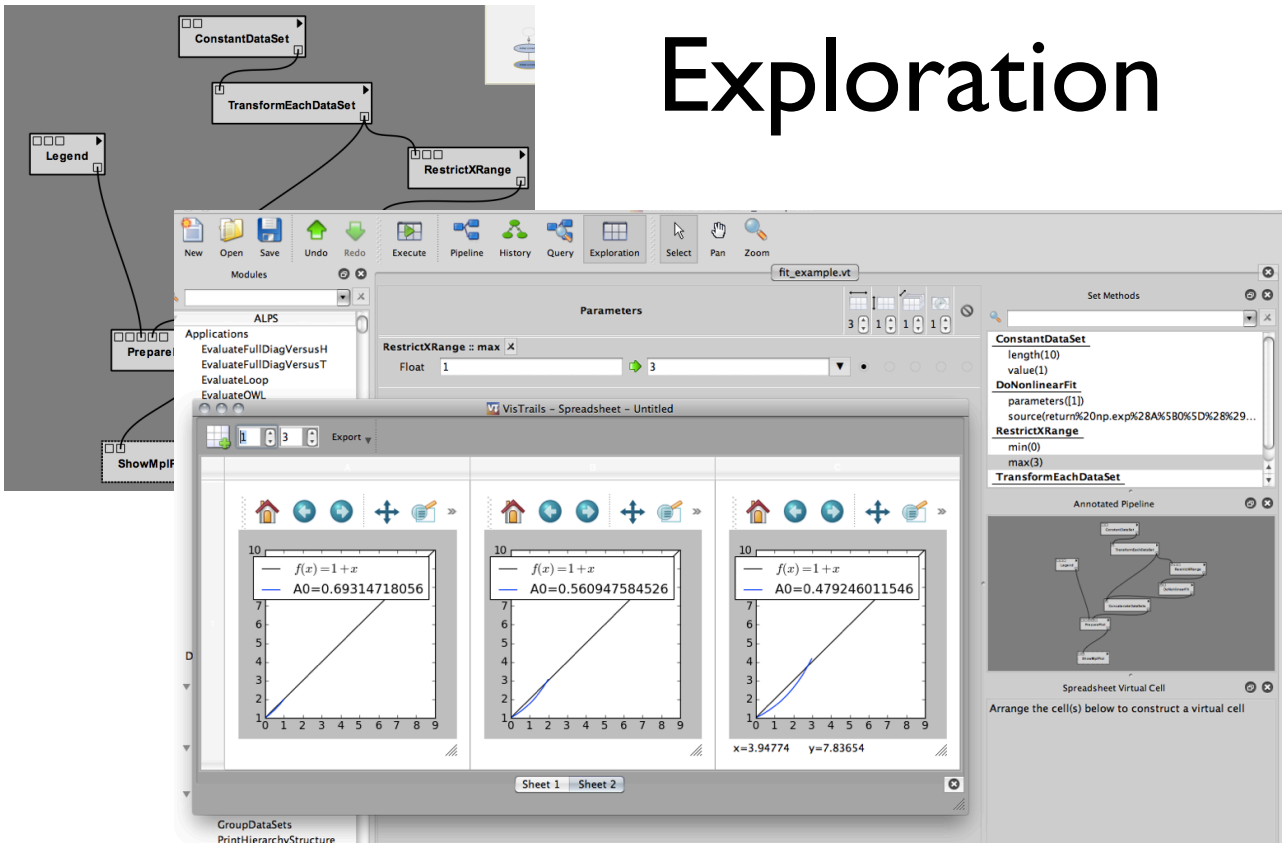
```
mins = {}
for ds in data:
    mins[ds[0].props[t]] = min([min(v.y) for v in ds])
```

- Functions for grouping/flattening, applying transformations at any level etc. exist

The spreadsheet



Exploration



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Odds and ends

- How to get more error messages on Mac? Try:
  `vispython /Applications/VisTrails/Vistrails.app/Contents/Resources/vistrails.py`
- Screencast introduction to VT and some DataSet modules: http://alps.comp-phys.org/static/screencast